OPT++

An Object-Oriented Toolkit for Nonlinear Optimization

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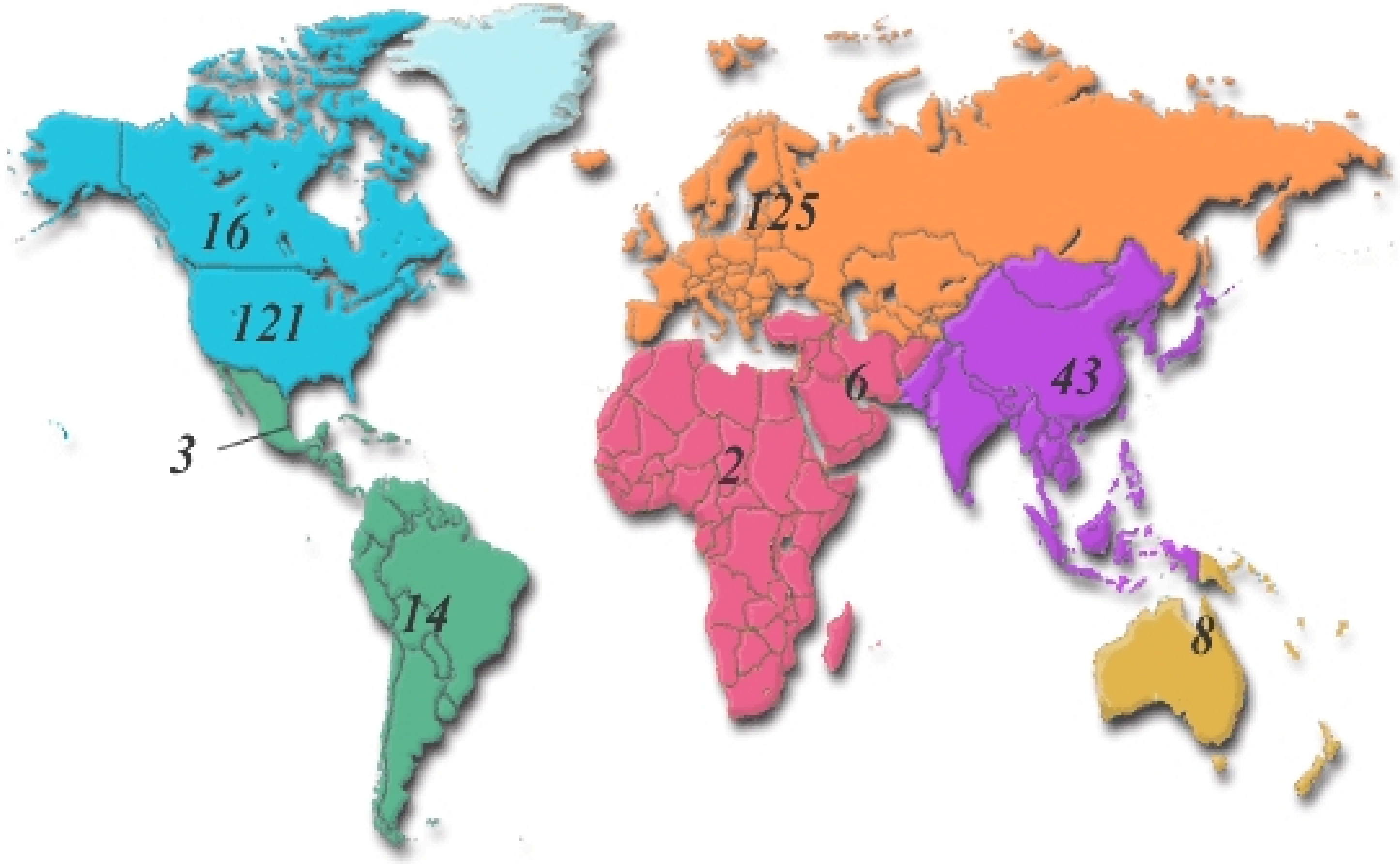
Outline

- Introduction to Optimization
- OPT++ Philosophy
- OPT++ Problem and Solver Classes
- Quick Tour of Algorithms
- Parallel optimization techniques
- Setting up a Problem and Algorithm
  - Example 1: Unconstrained Optimization
  - Example 2: Constrained Optimization
  - Example 3: Protein Folding
- Summary

Introduction

- OPT++ is an open source toolkit for general nonlinear optimization problems
- Original development started in 1992 at Sandia National Labs/CA
- Major contributors
  - Juan Meza, LBNL
  - Ricardo Oliva, LBNL
  - Patty Hough, SNL/CA
  - Pam Williams, SNL/CA

Global OPTimization

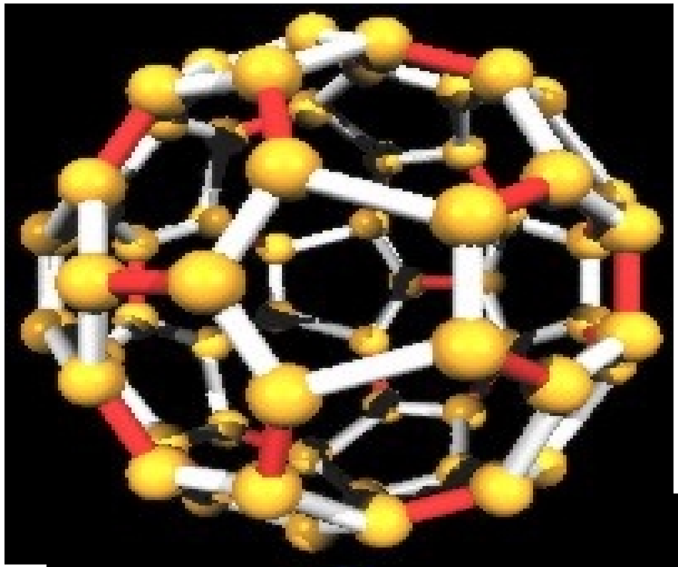


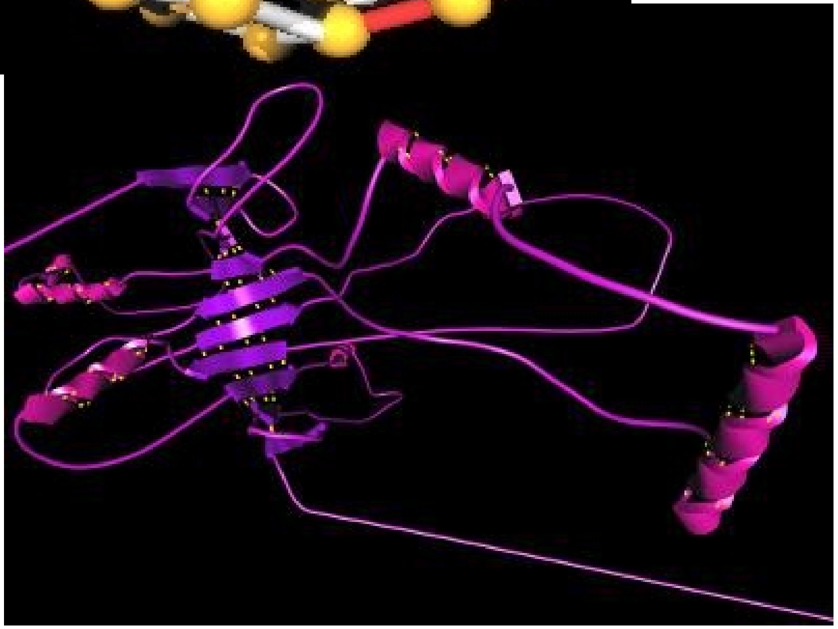
Total = 338

Other (Country not identified) = 120

As of April, 2003

Simulation-based optimization problems



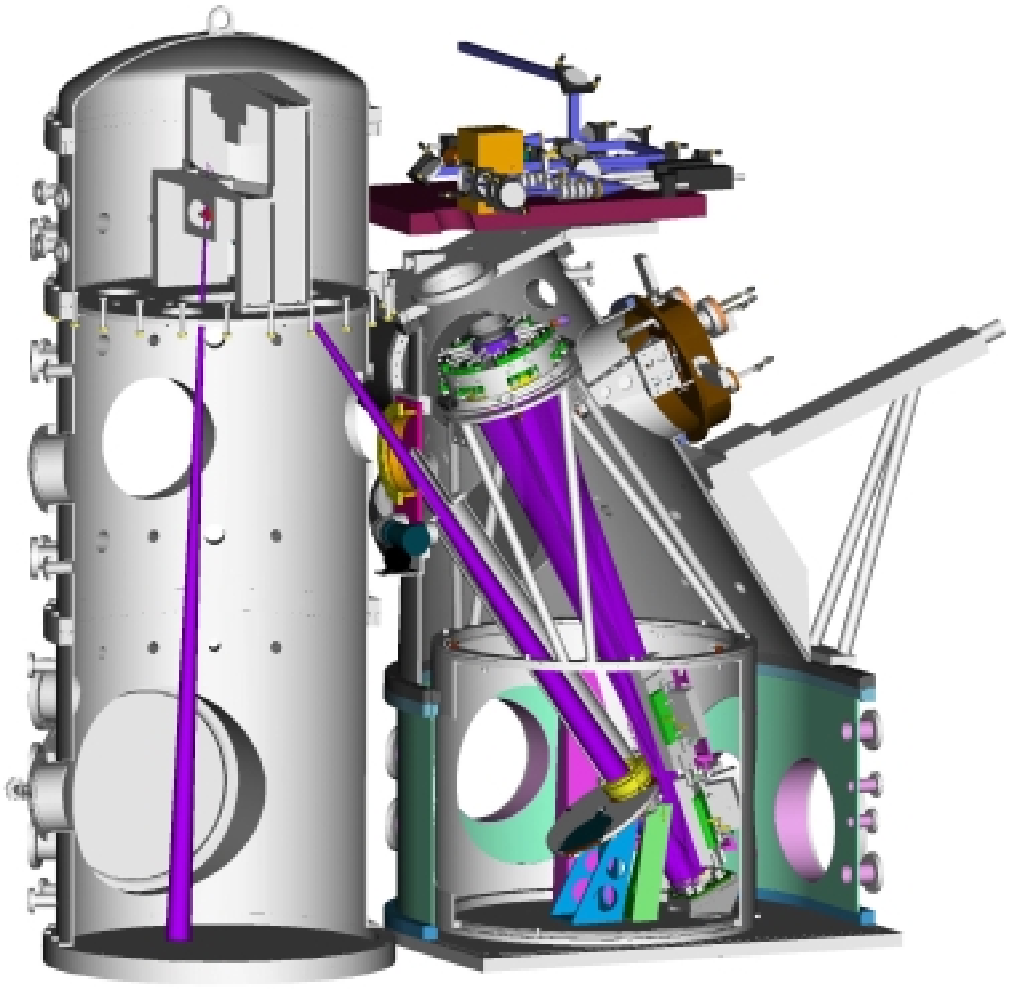


http://graphics.cs.ucdavis.edu/~okreylos/ResDev/ProtoShop/index.html

- Predict properties of nanostructures or design nanostructures with desired properties

- Protein folding problems: create secondary structures and obtain predictions of α-helices and β-sheets.

Parameter identification example

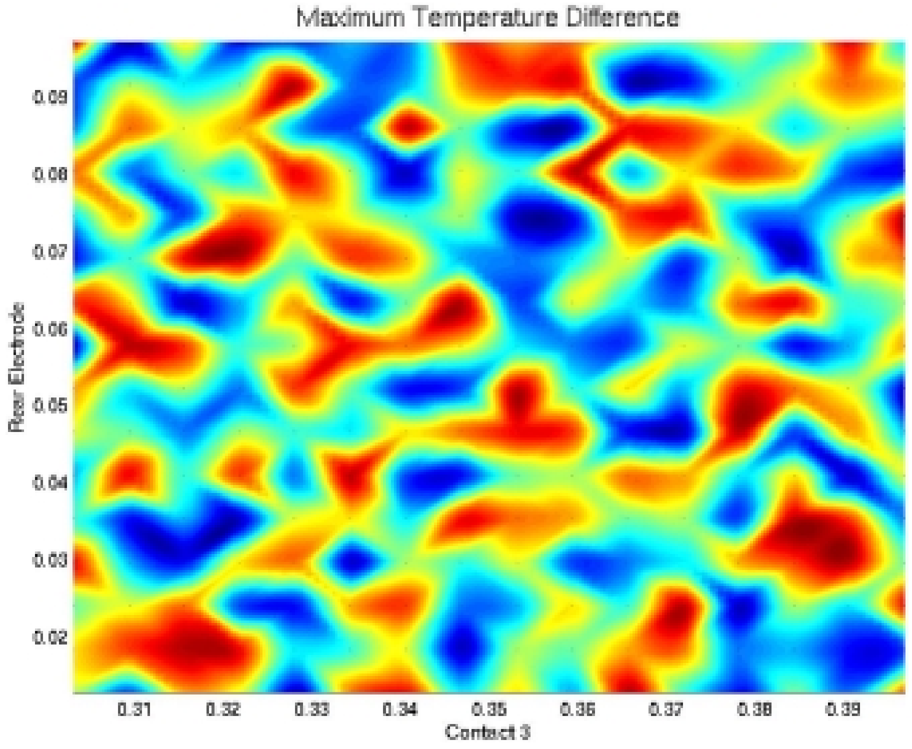


- Find model parameters, satisfying some bounds, for which the simulation matches the observed temperature profiles
- Computing objective function requires running thermal analysis code
- Each simulation requires approximately 7 hours on 1 processor

Formulation of parameter ID problem

$$\min_{x} \quad \sum_{i=1}^{N} (T_i(x) - T_i^*)^2$$

$$\text{s.t.} \quad 0 \le x \le u$$



- Objective function consists of computing the temperature difference between simulation results and experimental data
- Optimization landscape contains many local minima
- Uncertainty in both the measurements and the model parameters

General Optimization Problem

$$\min_{x \in \Re^n} f(x),$$ Objective function

$$s.t. \quad h(x) = 0,$$ Equality constraints

$$g(x) \geq 0$$ Inequality constraints

$$L = f(x) + y^T h(x) - w^T g(x)$$

Optimization Problem Types

- Unconstrained optimization
- Bound constrained optimization
  - Only upper and lower bounds
  - Sometimes called “box” constraints
- General nonlinearly constrained optimization
  - Equality and inequality constraints
  - Usually nonlinear
- Some special case classes (not currently handled in OPT++)
  - Linear programming (function and constraints linear)
  - Quadratic programming (quadratic function, linear constraints)

Some working assumptions

- Objective function is smooth
    - Usually true, but simulations can create noisy behavior
- Twice continuously differentiable
    - Usually true, but difficult to prove
- Constraints are linearly independent
    - Users can sometimes over-specify or incorrectly guess constraints
- Expensive objective functions

OPT++ Philosophy

- Problem should be defined in terms the user understands
  - *Do I have second derivatives available?* and not
  - *Is my objective function twice continuously differentiable?*
- Solution methods should be easily interchangeable
  - Once the problem is set up, methods should be easy to interchange so that the user can compare algorithms
- Common components of algorithms should be interchangeable
  - Algorithm developers should be able to re-use common components from other algorithms, for example line searches, step computations, etc.

Classes of Problems in OPT++

- Four major classes of problems available
  - *NLF0(ndim, fcn, init_fcn, constraint)*
    - Basic nonlinear function, no derivative information available
  - *NLF1(ndim, fcn, init_fcn, constraint)*
    - Nonlinear function, first derivative information available
  - *FDNLF1(ndim, fcn, init_fcn, constraint)*
    - Nonlinear function, first derivative information approximated
  - *NLF2(ndim, fcn, init_fcn, constraint)*
    - Nonlinear function, first and second derivative information available

Classes of Solvers in OPT++

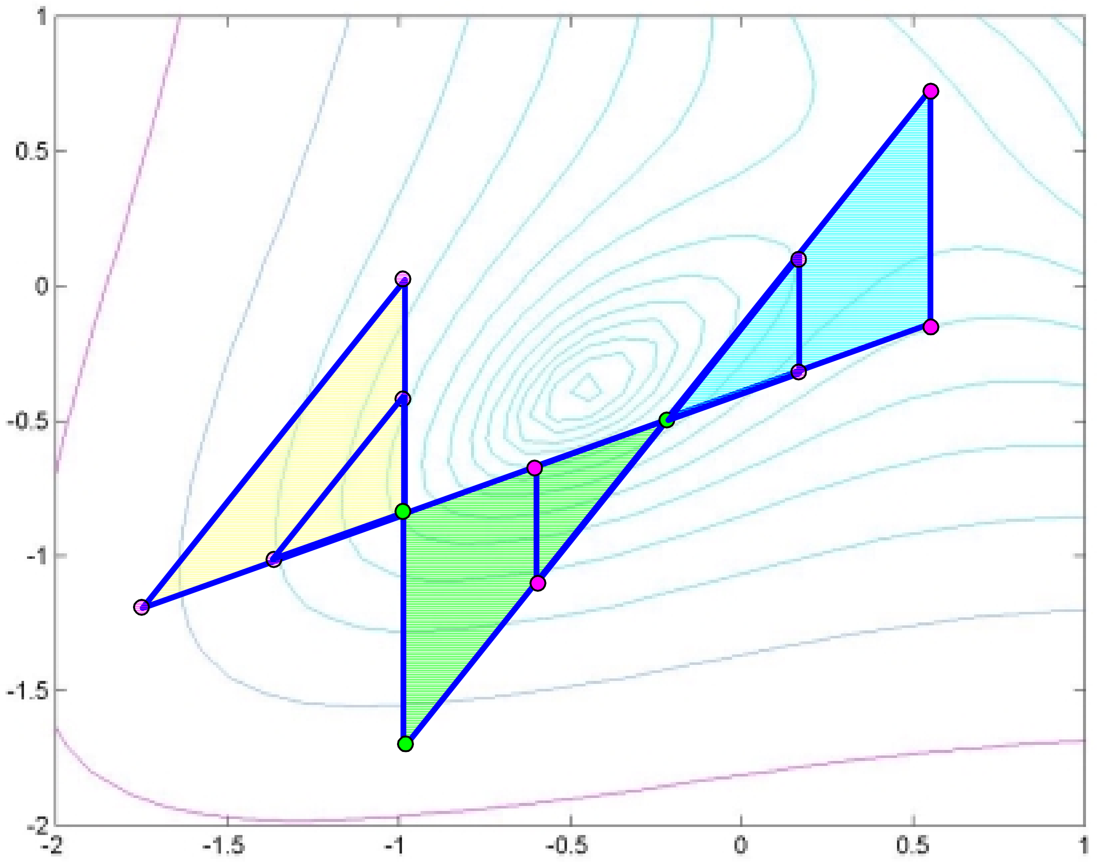
- Direct search
  - No derivative information required
- Conjugate Gradient
  - Derivative information may be available but doesn't use quadratic information
- Newton-type methods
  - Algorithm attempts to use/approximate quadratic information
  - Newton
  - Finite-Difference Newton
  - Quasi-Newton
  - NIPS

Constraints

- Constraint types
  - BoundConstraint(numconstraints, lower, upper)
  - LinearInequality(A, rhs, stdFlag)
  - NonLinearInequality(nlprob, rhs, numconstraints, stdFlag)
  - LinearEquation(A, rhs)
  - NonLinearEquation(nlprob, rhs, numconstraints)
- Everything combined
  - CompoundConstraint(constraints)

Quick tour of some of the algorithms

Pattern search

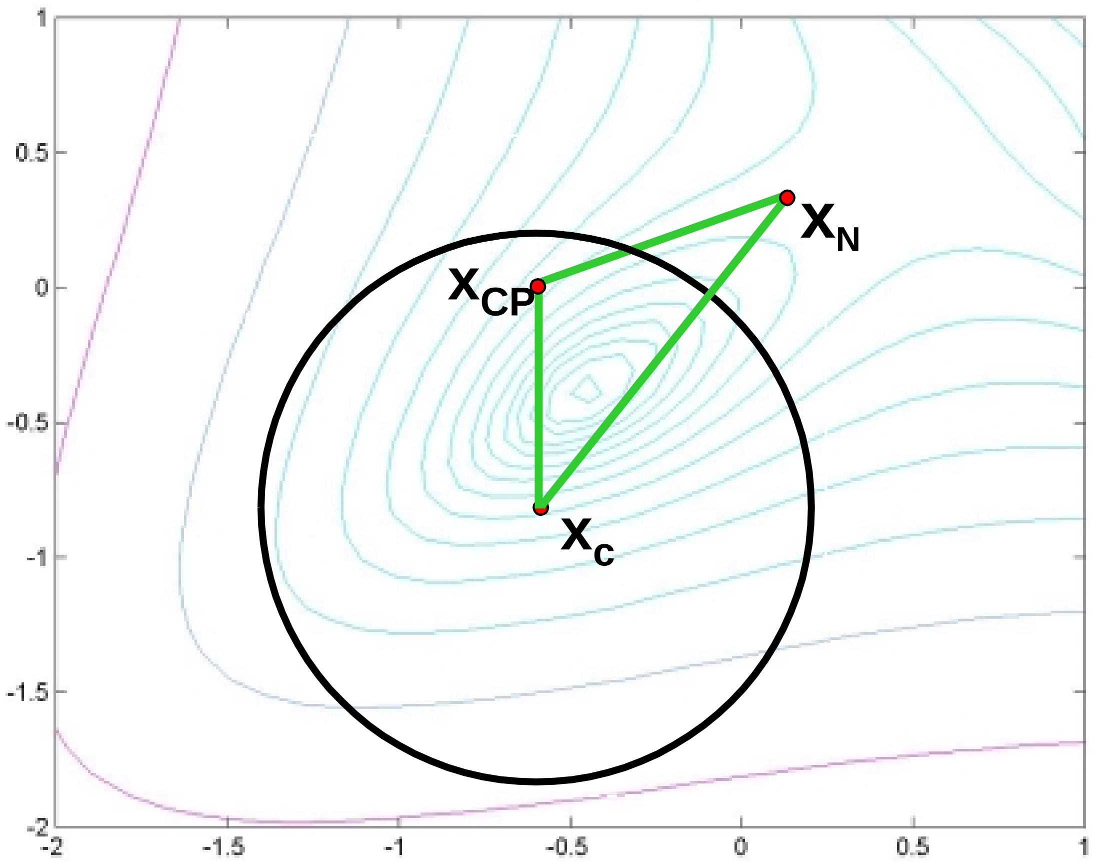


- Can handle noisy functions
- Do not require derivative information
- Inherently parallel
- Convergence can be painfully slow

Conjugate Gradient Methods

- Two major classes
- Standard nonlinear conjugate gradient
  - Two different types of line searches
- Limited Memory BFGS
  - Unconstrained version available
  - Bound constrained version under development

Newton-type Methods



- Fast convergence properties
- Good global convergence properties
- Inherently serial
- Difficulties with noisy functions

NIPS: Nonlinear Interior Point Solver

- Interior point method
- Based on Newton's method for a particular system of equations (perturbed Karush-Kuhn-Tucker, KKT, equations, slack variable form)
- Can handle general nonlinear constraints
- Can handle strict feasibility

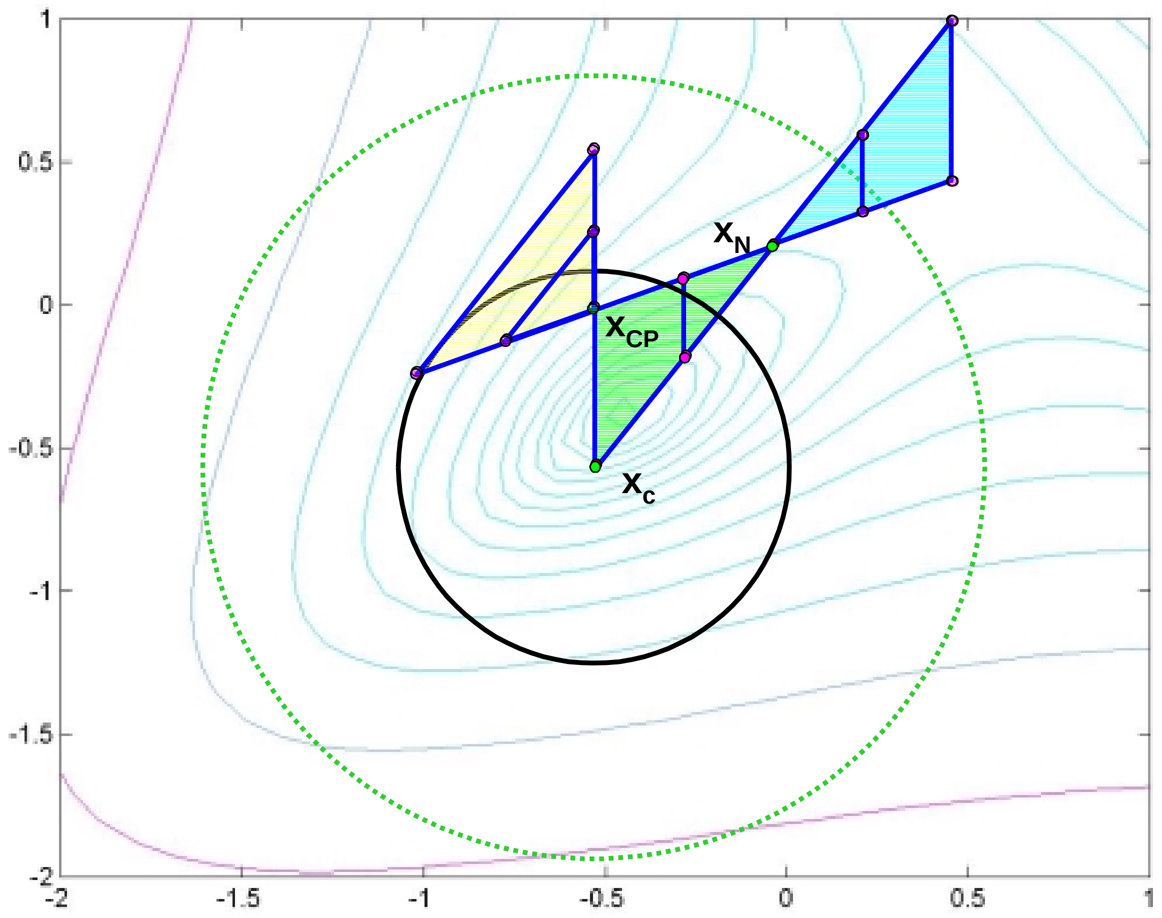
$$F(\mu) = \begin{bmatrix} \nabla f(x) + \nabla h(x) y - \nabla g(x) w \\ w - z \\ h(x) \\ g(x) - s \\ ZSe - \mu e \end{bmatrix} = 0$$

Parallel Optimization

Schnabel Identified Three Levels for Introducing Parallelism Into Optimization (1995)

- Parallelize evaluation of function/gradient/constraints
  - May or may not be easy to implement
- Parallelize linear algebra
  - Really only useful if the optimization problem is large-scale
- Parallelize optimization algorithm at a high level, for example, multiple function evaluations in parallel
  - Parallel Direct Search
  - Generalized Pattern Search
  - TRPDS

Trust Region + PDS



- Fast convergence properties of Newton method
- Good global convergence properties of trust region approach
- Inherent parallelism of PDS
- Ability to handle noisy functions

Algorithm Choices Depend on Problem

	NLF0	FDNLF1	NLF1	NLF2
OptPDS	x	x	x	x
OptCG		x	x	x
OptLBFGS		x	x	x
OptQNewton		x	x	x
OptBCQNewton		x	x	x
OptFDNewton		x	x	x
OptFDNIPS		x	x	x
OptNewton				x
OptBCNewton				x
OptNIPS				x

Example 1: unconstrained optimization

```
void init_rosen_x0(int ndim, ColumnVector& x);
void rosen(int ndim, const ColumnVector& x, double& fx, int& result);
int main() {
   int ndim = 2;
   FDNLF1 nlp(ndim, rosen, init_rosen_x0);
   nlp.initFcn();
   OptQNewton objfcn(&nlp);
   objfcn.setSearchStrategy(TrustRegion);
   objfcn.setMaxFeval(200);
   objfcn.setFcnTol(1.e-4);
   objfcn.optimize();
}
```

Example 2: Constrained optimization

$$\min\ (x_1 - x_2)^2 + (1/9)(x_1 + x_2 - 10)^2 + (x_3 - 5)^2$$

$$s.t.$$

$$x_1^2 + x_2^2 + x_3^2 \le 48,$$

$$-4.5 \le x_1 \le 4.5,$$

$$-4.5 \le x_2 \le 4.5,$$

$$-5.0 \le x_3 \le 5.0$$

Constrained optimization: Step 1

Defining the bound constraints:

$$-4.5 \le x_1 \le 4.5,$$
$$-4.5 \le x_2 \le 4.5,$$
$$-5.0 \le x_3 \le 5.0$$

```
int ndim = 3;

ColumnVector lower(ndim), upper(ndim);

lower << -4.5 << -4.5 << -5.0;

upper << 4.5 << 4.5 << 5.0 ;

Constraint bc = new BoundConstraint(ndim, lower, upper);
```

Constrained optimization: Step 2

Defining the nonlinear inequality constraint:

$$x_1^2 + x_2^2 + x_3^2 \leq 48$$

```
NLP* chs65 = new NLP(new NLF2(ndim, 1, ineq, init_hs65_x0));
Constraint nleqn = new NonLinearInequality(chs65);
```

Collecting both constraints into one constraint object :

```
CompoundConstraint* constraints =
                                        new CompoundConstraint(nleqn, bc);
```

Constrained optimization: Step 3

Defining and initializing the nonlinear problem:

```
NLF2 nips(ndim, hs65, init_hs65_x0, constraints);
nips.initFcn();
```

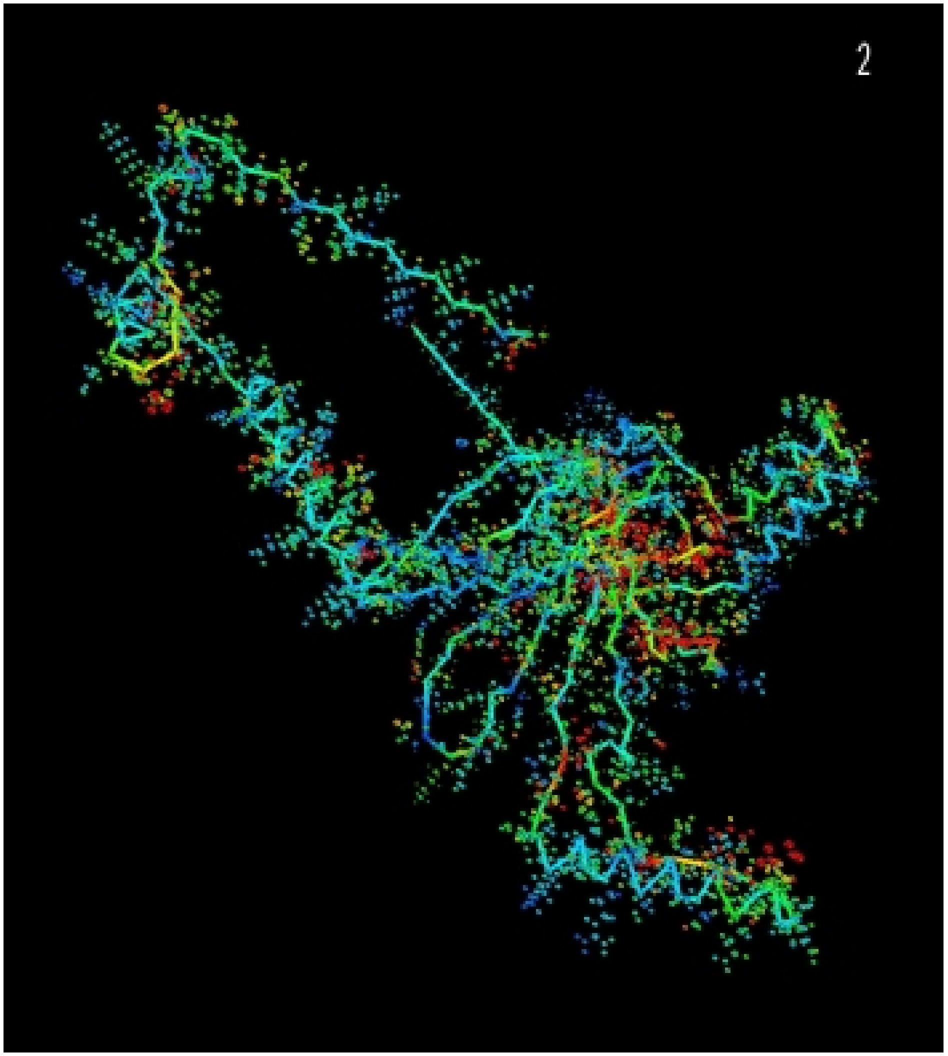
Defining the Optimization object and optimizing it!

```
OptNIPS optobj(&nips);
optobj.optimize();
```

Application: Protein Folding

```
void init_X0(int ndim, ColumnVector& x);
void eval_energy(int ndim, const ColumnVector& x, double& fx, int&
    result);
int main() {
    PDB pdb("t162.pdb");  // loads pdb file
    int ndim = 3 * pdb.NumAtoms();
    FDNLF1 nlp(ndim, eval_energy, init_X0);
    nlp.initFcn();
    OptLBFGS optobj(&nlp);
    optobj.setMaxFeval(10000);
    optobj.setFcnTol(1.e-6);
    optobj.optimize();
}
```

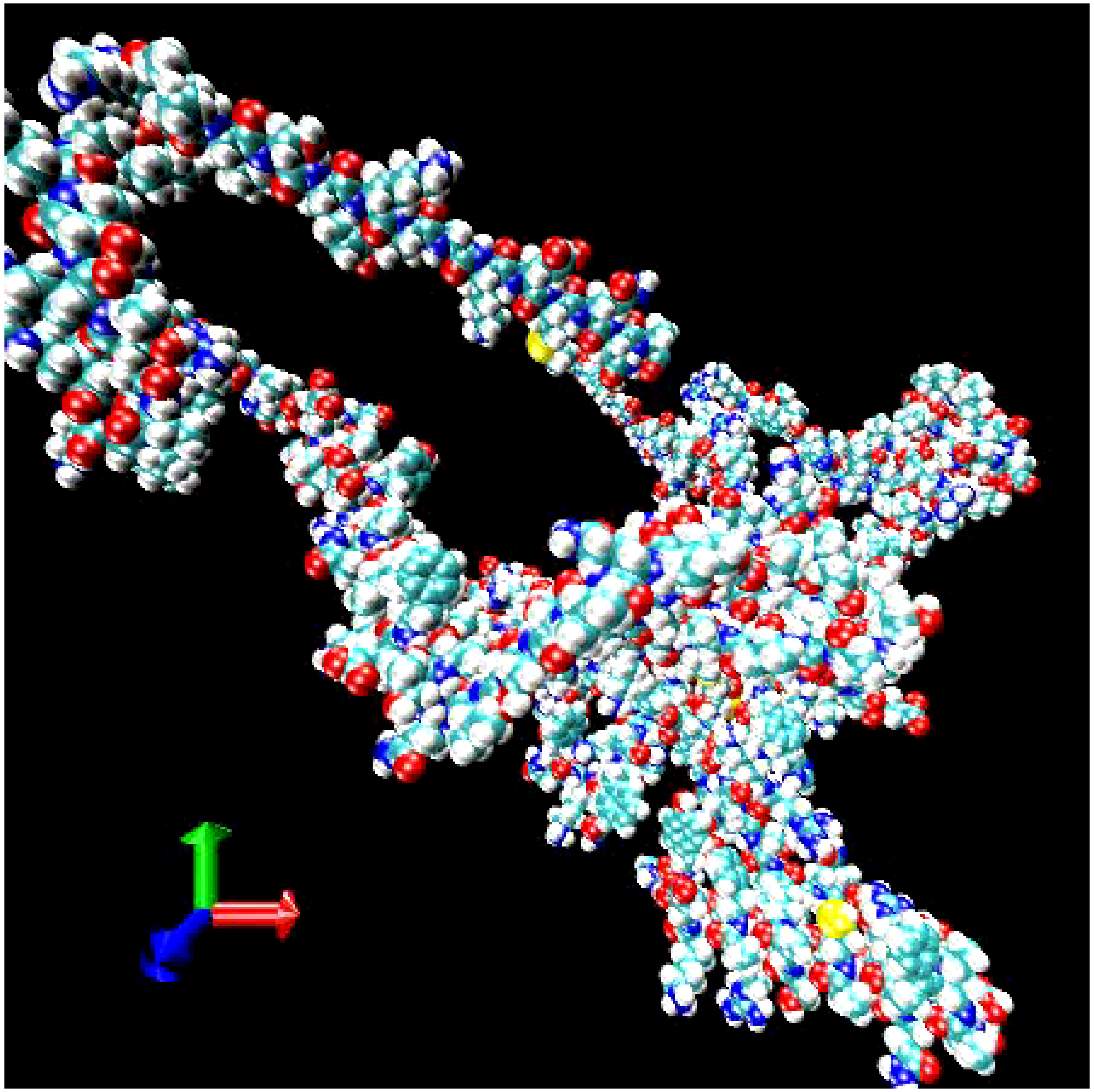
Energy Minimization Using LBFGS



- Energy Function: AMBER
- Protein 162;
- N = 13728 (4576 Atoms)
- LBFGS with M=15
- Total number of LBFGS iterations = 11656
- Total number of function evaluations = 11887
- Each function evaluation takes approximately 5 CPU sec

Protein T162 (from CASP5)

Protein T162 (from CASP5)



- Initial configuration created using ProteinShop (S. Crivelli)
- Energy minimization computed using OPT++/LBFGS
- Final average RMSD change was 3.9
- Total simulation took approximately 32 hours on a 1.7GHz machine with 512 RAM

Summary

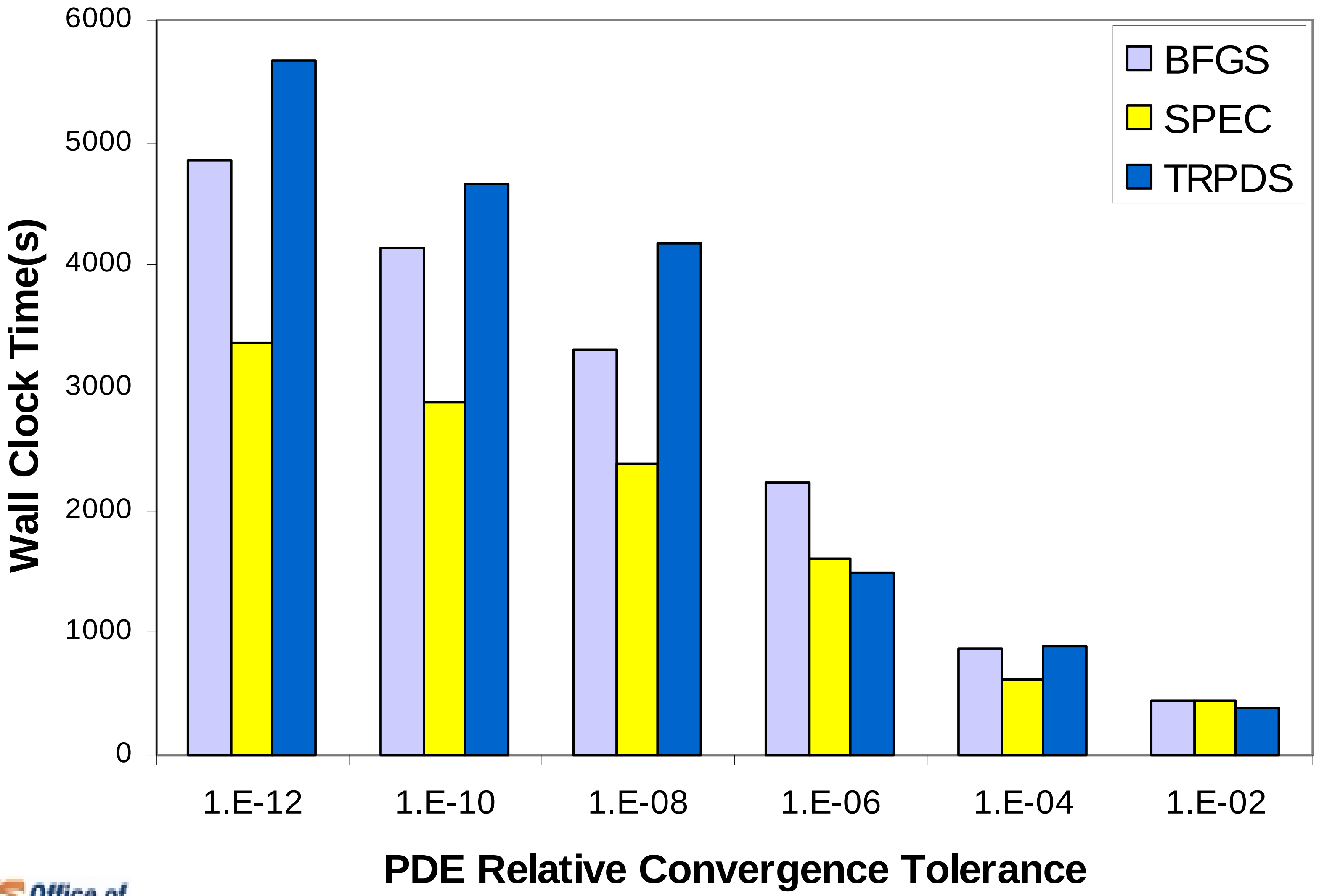
- OPT++ can handle many types of nonlinear optimization problems
- The toolkit can be used to compare the effectiveness of several algorithms on the same problem easily
- The user needs to provide only functions for the objective function and the constraints
  - If additional information is available it can be easily incorporated
- The code is open source and available at either
  - http://www.nersc.gov/~meza/projects/opt++
  - http://csmr.ca.sandia.gov/opt++

Backup Material

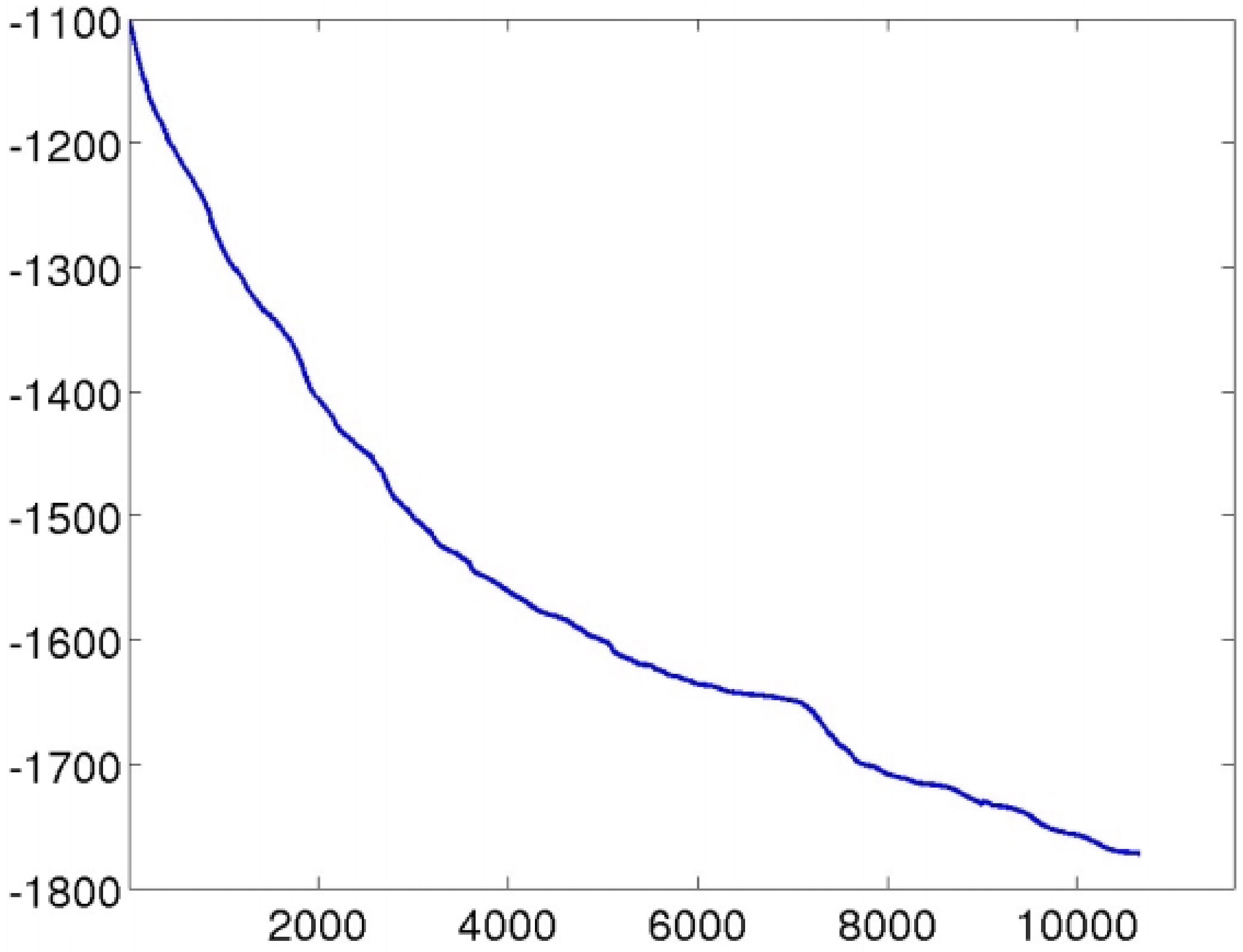
References

- Other links
  - http://sal.kachinatech.com/B/3/index.shtml
  - http://www-neos.mcs.anl.gov/neos
  - http://www.mcs.anl.gov/tao
  - http://endo.sandia.gov/DAKOTA/index.html
- Books/Papers
  - Dennis and Schnabel, *Numerical Methods for Unconstrained Optimization and Nonlinear Equations*, Prentice-Hall, 1983
  - Gill, Murray, Wright, *Practical Optimization*, Academic Press, 1981
  - El-Bakry, Tapia, Tsuchiya, Zhang, *On the Formulation and Theory of the Newton Interior-Point Method for Nonlinear Programming*, JOTA, Vol. 89, No.3, pp.507-541, 1996
  - More´ and Wright, Optimization Software Guide, SIAM, 1993

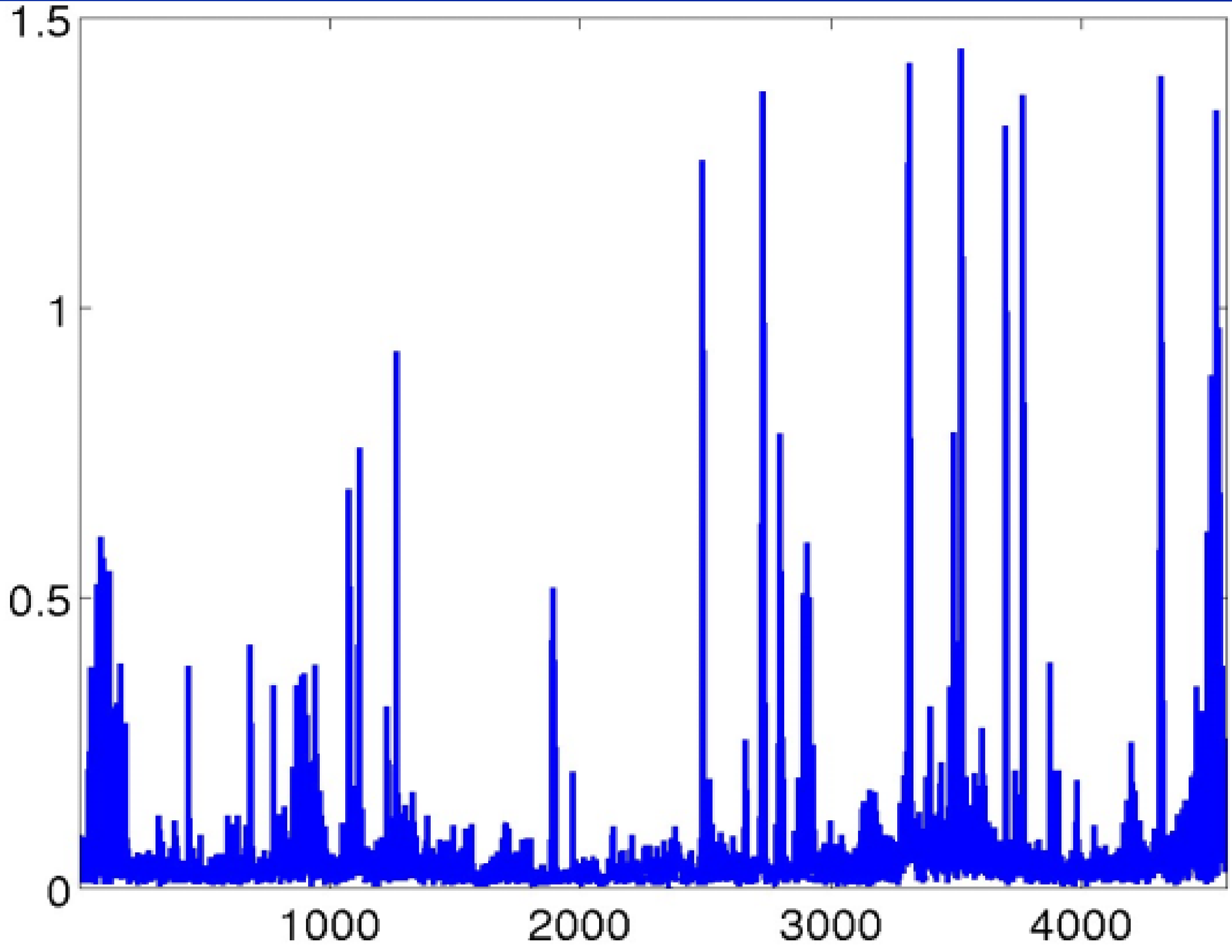
Comparison of TRPDS with other approaches



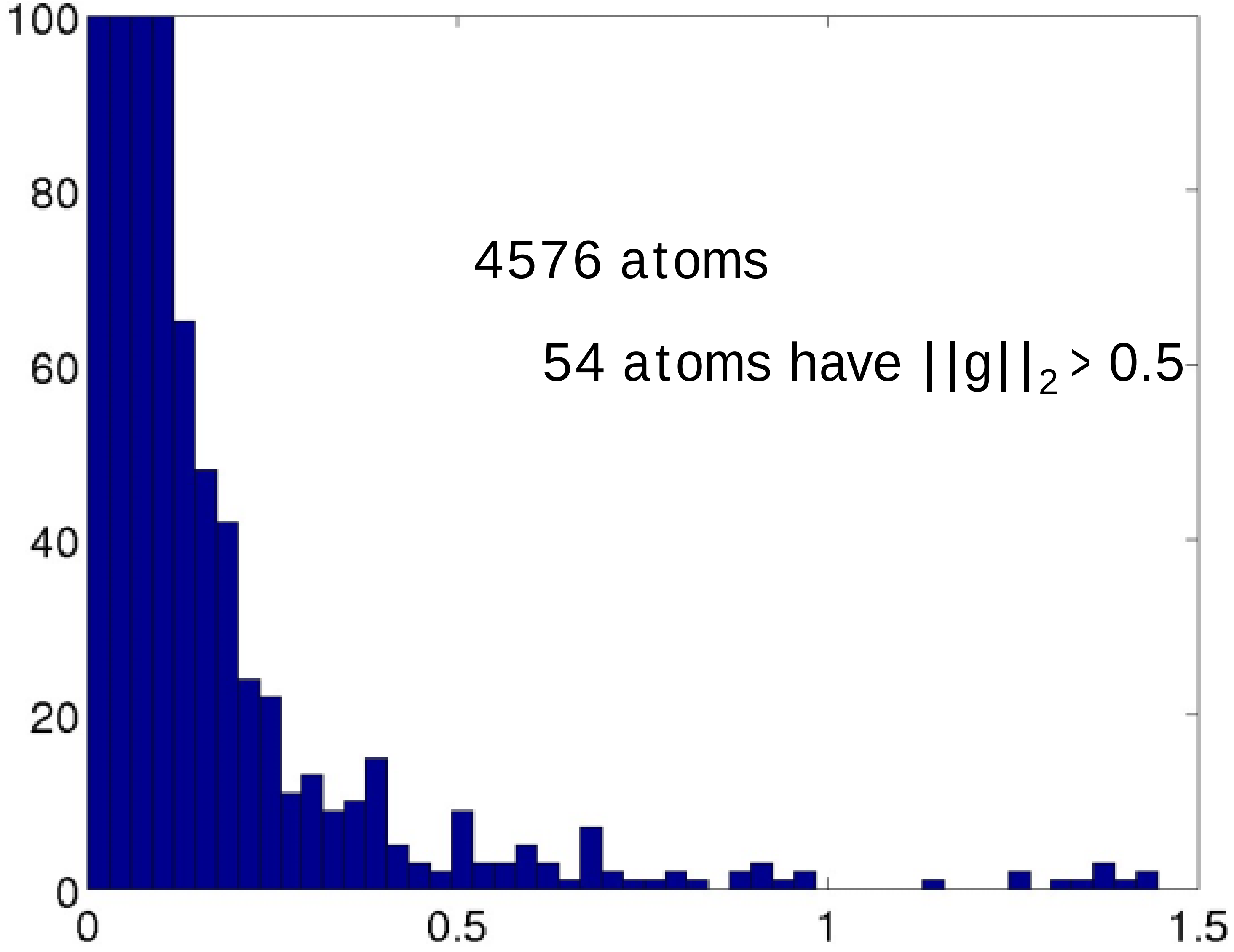
Energy vs. LBFGS iterations for T162 Problem



T162 Protein: ||gradient|| by atom



Distribution of ||gradient|| by atom



4576 atoms

54 atoms have $||g||_2 > 0.5$